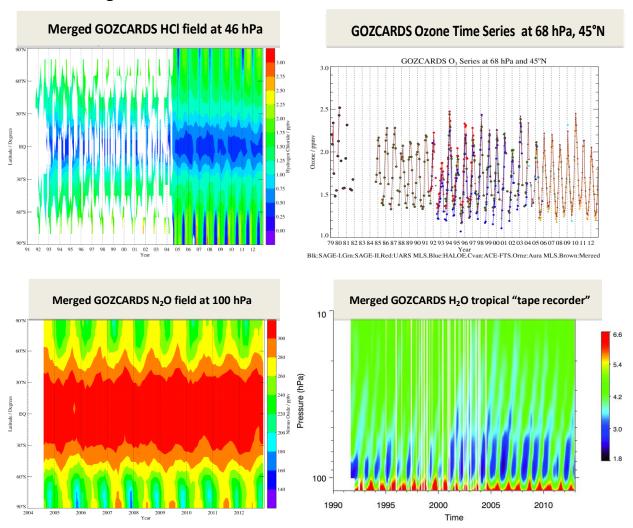


# National Aeronautics and Space Administration Goddard Earth Science Data Information and Services Center (GES DISC)

### **README Document** for the

Global OZone Chemistry And Related trace gas Data records for the Stratosphere (GOZCARDS) project

### **Zonal Average Pressure versus Latitude Time Series Products**



**Version 1.1** (Last Revised 4/2/2013)

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# **Revision History**

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# 1. Introduction

This document provides basic information for using the products from MEaSURES GOZCARDS (zonal average time series on pressure/latitude grid). This MEaSURES GOZCARDS ESDR consists of products generated with a focus on stratospheric ozone and related chemical species. The products include zonal average time series derived from "Level 2" products including stratospheric volume mixing ratio (VMR) and temperature profiles, based primarily on measurements from satellite-borne instruments, and largely from NASA missions studying the Earth's stratosphere since the late 1970s.

Users of these datasets should find that the concepts described below are fairly straightforward, and that the merged dataset results (time series in various latitude/pressure bins) match the source datasets being merged together, but for some additive offsets that mitigate data discontinuities (average biases) between the different instruments' measurements. Some caveats will also be included for each one of the GOZCARDS products, as they get delivered for public consumption, further validation, and potential updates and improvements in the future.

More technical details, examples, and validation will be submitted for publication (and also for website access) by the GOZCARDS project team soon after the delivery of GOZCARDS data products, as these become available, in sequence.

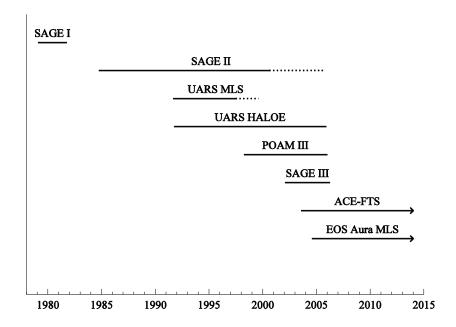
# 1.1 Data Product and Instrument Description

Table 1 below summarizes the GOZCARDS products (stratospheric species name or temperature (T)), and source datasets that were considered. The products files include source datasets (individual instrument records) as well as merged datasets, based on a combination of instruments. The product types in the GOZCARDS files are species Volume Mixing Ratio (VMR) or T time series on a latitude/pressure grid (10° zonal averages, typically monthly averages). If there are large data gaps between some measurement records, the merged (combined) data record may be identical or very similar (when adjustment guidelines can be provided) to the union of these records.

**Table 1.** Products and data sources considered for the creation of the MEaSURES GOZCARDS stratospheric ESDR. Not all datasets below are used when producing a merged product (a few datasets are used mainly for comparison/validation). Shown in blue are products with data files now publicly available from the NASA Goddard Earth Sciences and Information Services Center (GES DISC; see <a href="http://disc.gsfc.nasa.gov">http://disc.gsfc.nasa.gov</a>); these GOZCARDS datasets have ongoing measurements and analyses, and have been made available for time periods through 2012.

Products (and max. range of pressures)	Data Sources (and data years)
HCI (147 – 0.5 hPa)	HALOE (1991-2005), ACE-FTS (2004 onward), Aura MLS (2004 onward)
H <sub>2</sub> O (147 – 0.01 hPa)	HALOE (1991-2005), UARS MLS (1991-1993), ACE-FTS (2004 onward), Aura MLS (2004 onward)
O <sub>3</sub> (215 – 0.2 hPa)	SAGE I (1979-1981), SAGE II (1984-2005), HALOE (1991-2005), UARS MLS (1991-1997), ACE-FTS (2004-onward), Aura MLS (2004 onward) + others as validation (e.g., SAGE III, 2002-2005)
CIO (100 – 1 hPa)	UARS MLS (1991-1997), Aura MLS (2004 onward)
HNO₃ (215 – 1 hPa)	UARS MLS (1991-1997), ACE-FTS (2004 onward), Aura MLS (2004 onward)
HF (147 – 0.5 hPa)	HALOE (1991-2005), ACE-FTS (2004 onward)
N <sub>2</sub> O (100 – 0.5 hPa)	ACE-FTS (2004 onward), Aura MLS (2004 onward)
CH <sub>4</sub> (147 – 0.1 hPa)	HALOE (1991-2005), ACE-FTS (2004 onward)
CIO <sub>x</sub> (100 – 10 hPa)	UARS MLS (1991-1997), Aura MLS (2004 onward)
NO <sub>2</sub> (100 – 1 hPa)	SAGE II (1984-2005), HALOE (1991-2005), POAM III (1998-2005), SAGE III (2002-2005), ACE-FTS (2004 onward)
NO (100 – 1 hPa)	HALOE (1991-2005), ACE-FTS (2004 onward)
NO <sub>x</sub> (100 – 1 hPa)	SAGE II (1984-2005), HALOE (1991-2005), POAM III (1998-2005), SAGE III (2002-2005), ACE-FTS (2004 onward)
<b>Temperature</b> (1000 – 0.015 hPa)	GMAO MERRA (1979 onward)

Figure 1 below summarizes the timeline and names for the missions and instruments that have been considered/used for the generation of GOZCARDS products. A brief summary description for each instrument and measurement set is provided further below



**Figure 1.** Timeline of satellite missions and instruments considered for the GOZCARDS project and the creation of a stratospheric composition ESDR. Dotted lines indicate some degradation in coverage during the ending phase of some missions (SAGE II, UARS MLS); HALOE also suffered from poorer coverage in the second half of the UARS mission.

We provide below a list of the nine main data sources (instrument names or MERRA) for the creation of the GOZCARDS ESDR, along with a brief description, and electronic links to the original dataset locations.

### 1.1.1 SAGE I

The Stratospheric Aerosol and Gas Experiment I (SAGE I) was launched February 18, 1979, aboard the Applications Explorer Mission-B (AEM-B) satellite. SAGE I was a sun photometer that used solar occultation to measure aerosols and important stratospheric gases in the atmosphere. SAGE I collected valuable data for nearly three years until the power system on the satellite failed. SAGE I developed a global database for stratospheric aerosol, ozone, and nitrogen dioxide that is still used in the study of trends, atmospheric dynamics and transport, and potential climatic effects.

For more information and access to these data please go to:

### http://sage.nasa.gov/SAGE1

### 1.1.2 SAGE II

SAGE II (Stratospheric Aerosol and Gas Experiment II) was launched aboard the Earth Radiation Budget Satellite (ERBS) in October 1984. During each sunrise and sunset encountered by the orbiting spacecraft, the instrument used the solar occultation technique to measure stratospheric aerosols, ozone, nitrogen dioxide, and water vapor.

SAGE II continued the SAGE measurements of stratospheric ozone from 1984-2005. This long-term, stable data set has proven very valuable in determining trends in ozone.

For more information and access to these data please go to:

### http://sage.nasa.gov/SAGE2

### 1.1.3 SAGE III

SAGE III-Meteor-3M was a third generation, satellite-borne instrument and a crucial element in NASA's Earth Observing System (EOS). The instrument was launched on the Russian Meteor-3M spacecraft in December 2001. The Meteor-3M mission was terminated on March 6, 2006, because of a power supply system failure resulting in loss of communication with the satellite.

The SAGE III mission enhanced our understanding of natural and human-derived atmospheric processes by providing accurate measurements of the vertical structure of aerosols, ozone, water vapor, and other important trace gases in the upper troposphere and stratosphere.

For more information and access to these data please go to:

### http://sage.nasa.gov/SAGE3M3M

### **1.1.4 HALOE**

Since its launch on September 12, 1991 from the Space Shuttle Discovery, the Halogen Occultation Experiment (HALOE) collected profiles of middle atmosphere composition and temperature on board the Upper Atmosphere Research Satellite (UARS). HALOE used solar occultation to measure simultaneous vertical profiles of ozone (O<sub>3</sub>), hydrogen chloride (HCl), hydrogen fluoride (HF), methane (CH<sub>4</sub>), water vapor (H<sub>2</sub>O), nitric oxide (NO), nitrogen dioxide (NO<sub>2</sub>), temperature, aerosol extinction at 4 infrared wavelengths, aerosol composition and size distribution versus atmospheric pressure with a 1.6 km instantaneous field of view at the Earth's limb. HALOE collected data from October 11, 1991 until November 11, 2005.

For more information and access to these data please go to:

### http://disc.sci.gsfc.nasa.gov/UARS/data-holdings/HALOE

### **1.1.5 UARS MLS**

The Microwave Limb Sounder (MLS) was one of 10 instruments aboard the Upper Atmosphere Research Satellite (UARS). The instrument had three radiometers, at frequencies near 63, 183 and 205 GHz. The major objective of UARS MLS was to provide global information on chlorine monoxide (ClO), the dominant form of chlorine that destroys ozone. UARS MLS was also designed to measure stratospheric ozone and water vapor. Additional measurements were obtained, including: stratospheric temperature, upper tropospheric water vapor, cloud ice water content, stratospheric HNO<sub>3</sub>, volcanic SO<sub>2</sub> injected into the stratosphere, temperature variances associated with atmospheric gravity waves, and stratospheric CH<sub>3</sub>CN.

UARS MLS generally provided daily measurements from September 19, 1991 through March 15, 1994, although stratospheric water vapor measurements ceased on April 15, 1993 due to the failure of the 183 GHz radiometer. After March 15, 1994 the measurements became increasingly sparse in order to conserve the life of the MLS antenna scan mechanism and UARS power. Data are available through July 28, 1999, although for GOZCARDS, only data through mid-June, 1997, are considered (failure of the 63 GHz radiometer led to slightly less 'trend-quality' data after this time).

For more information and access to these data please go to:

http://disc.sci.gsfc.nasa.gov/UARS/data-holdings/MLS

### 1.1.6 Aura MLS

The Earth Observing System (EOS) Microwave Limb Sounder (MLS) is one of four instruments on the NASA's EOS Aura satellite, launched on July 15th 2004. Aura MLS is a greatly enhanced version of the UARS MLS experiment, providing better spatial coverage and vertical resolution. The instrument includes four radiometers at 118, 190, 240, and 640 GHz, and a 2.5 THz module. MLS provides measurements of many chemical species (O<sub>3</sub>, H<sub>2</sub>O, OH, HO<sub>2</sub>, HCl, HOCl, ClO, N<sub>2</sub>O, HNO<sub>3</sub>, CO, BrO, HCN, CH<sub>3</sub>CN, and volcanic SO<sub>2</sub>), cloud ice, temperature and geopotential height. The instrument has been making measurements continuously since August 2004, with the exception of OH which ceased regular (daily) measurements in August 2010 in order to preserve the life of the THz module.

For more information and access to these data please go to:

http://disc.sci.gsfc.nasa.gov/Aura/data-holdings/MLS/

### 1.1.7 ACE-FTS

The Atmospheric Chemistry Experiment mission's Fourier Transform Spectrometer (ACE-FTS) is the primary instrument onboard the SCISAT satellite. FTS is a high spectral resolution ( $0.02~\text{cm}^{-1}$ ) Fourier Transform Spectrometer (FTS) operating from 2.2 to 13.3  $\mu$ m (750-4400 cm<sup>-1</sup>) with a Michelson interferometer. The instrument is designed to simultaneously measure temperature, trace gases, thin clouds, and aerosols found in the atmosphere using the solar occultation technique.

For access to these data please go to:

http://www.ace.uwaterloo.ca

### 1.1.8 POAM III

The Polar Ozone and Aerosol Measurement III (POAM III) instrument was launched aboard the French SPOT-4 spacecraft in March 24, 1998. This instrument measured the vertical distribution of atmospheric ozone, water vapor, nitrogen dioxide, and aerosol extinction using the solar occultation technique. POAM III was operational until December 5, 2005. POAM III was an improved version of POAM II. It had an improved electronic system that provided lower noise and more accurate measurements. The optical filters were manufactured with a better technology that yields higher transmission and greater ability to withstand the space environment. The wavelengths and bandwidths of the science channels differed slightly from those in POAM II.

For access to these data please go to:

http://wvms.nrl.navy.mil/POAM

### 1.1.9 MERRA

The Modern-Era Retrospective Analysis for Research and Applications, or MERRA, is a NASA reanalysis for the satellite era using a major new version of the Goddard Earth Observing System Data Assimilation System Version 5 (GEOS-5). The Project focuses on historical analyses of the hydrological cycle on a broad range of weather and climate time scales and places the NASA EOS suite of observations in a climate context.

For access to MERRA data please go to:

http://disc.sci.gsfc.nasa.gov/mdisc/data-holdings/merra

For more information about MERRA data, please see <a href="http://gmao.gsfc.nasa.gov/merra">http://gmao.gsfc.nasa.gov/merra</a> and *Rienecker et al.* (2011). See also section 1.2.9 for the GOZCARDS-relevant application.

### 1.2 Data Versions and Validation References

The data versions used for GOZCARDS are provided as part of the data records (source files and merged files). Unless otherwise specified in the files, the following algorithm/data versions were used from the original source datasets ("Level 2 files", or "Level 3AT files" in the case of UARS MLS), after appropriate data profile screening (and/or outlier value screening) procedures. Note that some of the above datasets (SAGE III and POAM III in particular) have not been merged as part of the current (or now planned) GOZCARDS data record, due in part to logistical reasons, and as the main benefits for a merged product come from robust and long global time series (for "early" and "late" time periods within a data record); however, some datasets can be used as cross-checks, even if they are not used directly as part of the generation of a merged product.

A brief synopsis of validation-related references for the main species and datasets is provided below, focusing initially on HCl,  $O_3$ ,  $H_2O$ , ClO, and  $HNO_3$  (as the first phase of planned GOZCARDS deliveries). Note, however, that published validation papers do not always refer to the latest data versions, although changes in abundances between data versions are generally fairly small in the late stages of satellite missions. More detailed GOZCARDS-related information will be made available in GOZCARDS-related publication(s) and other (future) documentation.

### 1.2.1 SAGE I

Version 5.9\_rev is used. It was known that there were altitude errors in the original SAGE-I (V5.9) data (*Veiga et al.*, 1995, *Wang et al.*, 1996). An empirical altitude correction method based on *Wang et al.* (1996) had been applied to SAGE-I V5.9 ozone data before being used for GOZCARDS. This empirically corrected SAGE-I dataset (V5.9\_rev) had been evaluated and used in previous ozone trend studies (e.g. *SPARC Report*, 1998, *WMO*, 2003). The SAGE science team is working on a new retrieval algorithm to correct this altitude registration problem, which could potentially improve SAGE I ozone data in the lower stratospheric and upper tropospheric regions.

### 1.2.2 SAGE II

Version 6.2 is used. For ozone-related validation, see *Wang et al.* (2002), as well as *Wang et al.* (1996). However, the SAGE II  $H_2O$  version 6.2 data product (see *Taha et al.*, 2004, as a validation reference) was not included in the GOZCARDS merged result. This was decided after consideration of the resulting time series and the concerns of the SAGE II team itself regarding a channel drift issue (see *Thomason et al.*, 2004; also, *L. Thomason, private communication*). While there is value in attempting to extend the  $H_2O$  time series back in time to 1984 from the HALOE

starting date (in late 1991), some of the lower stratospheric H<sub>2</sub>O variations in the mid-1980's do not appear very robust; given the channel drift issue as well as data gaps and potential lower stratospheric artifacts from aerosol contamination as a result of the 1984 volcanic El Chichon eruption, the GOZCARDS team chose the conservative approach (not to use SAGE II H<sub>2</sub>O data at all). Also, the SAGE II H<sub>2</sub>O dataset becomes significantly noisier above the 3 hPa level. It may be that the recently produced version 7 SAGE II dataset will prove more robust and enable a a longer-period reconstruction of global H<sub>2</sub>O time series.

### **1.2.3 SAGE III**

Version 4.0 is used. However, this dataset is not part of the planned initial release for the GOZCARDS merged ozone product, but SAGE III ozone source data files have been created for the GOZCARDS record and this dataset can be used as a cross-check. See *Wang et al.* (2006) as well as *Kar et al.* (2007) for references related to SAGE III ozone.

### **1.2.4 HALOE**

Version 19 is used. See the following validation-related references: Russell et al. (1996) for HCl, Harries et al. (1996) and Taha et al. (2004) for  $H_2O$ , Brühl et al. (1996), Bhatt et al. (1999), and Randall et al. (2003) for  $O_3$ ; Grooß and Russell (2005) provided a useful reference for HALOE-derived climatologies and uncertainties. Hervig et al. (1995) and Hervig and McHugh (1999) developed screening criteria for the HALOE data, to account for contamination by aerosols, clouds, and tropospheric water vapor. These data screening criteria have undergone certain refinements over the years, including recently.

### **1.2.5 UARS MLS**

Version 5 is used for  $O_3$  and CIO, and version 6 is used for  $HNO_3$  and (stratospheric)  $H_2O$ . See *Livesey et al.* (2003) and references therein for more details. Version 6 for  $H_2O$  (from the GES DISC) is the same as the original prototype version (0104) (see *Pumphrey*, 1999). For brevity, UARS MLS is also referred to as UMLS in other portions of this document and in the relevant GOZCARDS file naming conventions.

### 1.2.6 Aura MLS

Version 2.2 is used for ozone and version 3.3 is used for other species. A set of validation papers was produced in 2007 and 2008 for version 2.2; see Froidevaux et al. (2008a), Jiang et al. (2007), and Livesey et (2008)for O<sub>3</sub>, Froidevaux et al. (2008b)for HCl, Lambert et al. (2007) for stratospheric H<sub>2</sub>O and for N<sub>2</sub>O, Read et al. (2007) and Vömel et al. (2007) for upper tropospheric/lower stratospheric H<sub>2</sub>O, Santee et al. (2007) for HNO<sub>3</sub>, and Santee et al. (2008) and Connor et al. (2007) for CIO. See also Manney et al. (2007) for non-coincident validation studies. Some updates regarding version 3.3 data validation have been provided in the Aura MLS data quality documentation (*Livesey et al.*, 2011). Also, *Nedoluha et al.* (2011) have provided cross-validation results tying the ground-based ClO measurements to the MLS ClO data from both UARS and Aura. For brevity, Aura MLS is also referred to as AMLS in other portions of this document and in the relevant GOZCARDS file naming conventions.

### **1.2.7 ACE-FTS**

Version 2.2 update is used for ozone, and the standard version 2.2 is used for the other ACE-FTS species that are included in GOZCARDS. The main ACE-FTS (version 2.2) validation references for some of the GOZCARDS-related species are by *Mahieu et al.* (2008) for HCl and HF, *Carleer et al.* (2008) for H<sub>2</sub>O, and *Dupuy et al.* (2009) for O<sub>3</sub>, and *Wolff et al.* (2008) for HNO<sub>3</sub>; see also *Hegglin et al.* (2008) for non-coincident validation studies of ACE-FTS data (for O<sub>3</sub>, H<sub>2</sub>O, and CO) in the upper troposphere/lower stratosphere (UTLS).

Notes: Data processing issues for ACE-FTS v2.2 data have led us to limit the ACE-FTS datasets to dates prior to and including the last day of September, 2010 for species other than ozone; for ozone, we have limited the (v2.2 update) data to dates prior to and including the last day of December, 2009. The first ACE-FTS data month recommended for use is March, 2004; for N2O and HNO3, we start the current merged datasets combining Aura MLS and ACE-FTS data on the same month, namely August 2004, when the MLS retrievals started. These issues could be remedied in the future through the use of version 3 data, or by using updated version 2 data from the ACE-FTS team, so that dates after the above limiting dates could be included as well for GOZCARDS.

### 1.2.8 POAM III

Version 4.0 is the latest data release for POAM III. Note that this dataset has not been merged as part of the GOZCARDS record, mainly due to logistical reasons, and as the main benefits for merging come from more global time series. See *Randall et al.* (2003) and references therein as a validation reference for POAM III ozone and *Lumpe et al.* (2006) for H<sub>2</sub>O.

### **1.2.9 MERRA**

The MERRA temperature fields used for GOZCARDS are from the DAS 3d analyzed state MAI6NVANA, version 5.2.0 (files such as MERRA300.prod.assim.inst6\_3d\_ana\_Nv.20110227.hdf). In brief, temperature data from 4 daily files (for 00, 06, 12, and 18 hr UT) are averaged to provide daily mean fields (appropriate for a mean time of 09 hr). Interpolation is performed onto the fixed GOZCARDS pressure grid (30 pressures levels from 1000 to 0.0147 hPa). Averaged values

are stored for the 10° GOZCARDS latitude bins; daily results are binned into a monthly average for the GOZCARDS monthly files.

# 1.3 Algorithm Background

The basic elements of the algorithms relating to the GOZCARDS records are described briefly below. Note that each species often has its own specific set of issues, often relating to the specific instrument measurements, sampling, and measurement overlap periods or regions available; case-by-case considerations and further details will be described elsewhere (the GOZCARDS team is planning manuscripts for the peer-reviewed literature).

In general, if one considers several measurement systems for a given species as a function of time, the GOZCARDS algorithm is based on the use of the overlapping time periods between the various measurements to define additive offsets and remove the instrument-to-instrument biases; as a result, with enough overlap time and high quality, properly screened data, one can obtain a merged time series. The offsets between the various measurements are determined by comparing the monthly mean values during overlap and by adjusting to an average reference.

We provide some more information below on the procedures that were used for merging datasets for various species. We have limited some datasets for the merging process when it was clear that significant biases versus other datasets exist; for example, UARS MLS ozone data at 100 hPa in the tropics have a clear high bias (by more than 50%) versus HALOE and SAGE II ozone, so the UARS MLS data at this pressure for the 25°S through 25°N latitude bins was not included in the merging process. We also tend to ignore ozone data that are clearly in the upper troposphere for this GOZCARDS project, geared towards the stratosphere. More validation would probably be needed and less data continuity (for long time series) exists anyway in the upper troposphere. Ozone data extend down to the 215 hPa pressure level at high latitudes, but only to 100 hPa in the tropics. Similarly, the water vapor data are largely stratospheric, given the 147 hPa pressure chosen as the bottom of this merged dataset. For some species (like N₂O and HNO<sub>3</sub>), the lower boundary is determined by the Aura MLS lowest boundary, and we have preferred to keep the continuity of the dataset in terms of coverage tied to the Aura MLS data; some extension could be performed (by data users) by using ACE-FTS N2O down to 147 or 215 hPa (and by using the same offset values as provided in the data files at 100 hPa), but significant data gaps would exist compared to the 100 hPa level. Also, the N<sub>2</sub>O and HNO<sub>3</sub> datasets start in August 2004, when Aura MLS monthly data started; a small extension in time could be obtained by using ACE-FTS data during the few months prior to August 2004, when ACE-FTS data exist, but again, with some break in the data continuity. For the longer time series such as O<sub>3</sub>, H<sub>2</sub>O, and HCl, we simply maintain the differences in sampling frequency versus time; what can look like significant differences in seasonal cycles is usually caused by these differences in sampling frequencies between occultation instruments (which span the globe in about a month) and the (daily global) emission measurements by MLS instruments. Future analyses of these data records could lead to the benefit of 'reanalyzed' data records with data gaps filled in, although there are various ways of doing this; this, however, is one step further removed from the actual datasets, and is not the goal (nor within the bounds) of this GOZCARDS work.

### HCl and H<sub>2</sub>O

For HCl and H<sub>2</sub>O, the overlap period between the March 2004 (first available/recommended) ACE-FTS monthly means and the November 2005 last useful set of HALOE data is used to determine a reference based on the average of all three datasets available, which includes Aura MLS (start of MLS data is August, 2004). In reality, the averaging does not use the set of data values that are exactly collocated in time, as there is often only a small number of such values; instead, Aura MLS (AMLS) data are used as a transfer standard, as this dataset has essentially continuous time/space coverage. An iterative procedure is used for the merging process in each latitude/pressure bin. First, collocated AMLS and ACE-FTS values are averaged in the Aug. 2004 to Dec. 2005 time period to obtain an average reference (labeled ref1); the full original time series from ACE-FTS and AMLS are then offset (by the appropriate opposite and equal amounts) and merged (averaged), wherever they both provide a monthly mean value. Then, the HALOE data values are adjusted by using as a new reference the above previously-adjusted AMLS/ACE-FTS combination. The new average reference is constructed from the average collocated set: ref2 value =  $(1/3)x(HALOE \ value) + (2/3)x(ref1 \ value)$ , and this is used to produce new average offsets and correspondingly-adjusted series, which are then merged (averaged) together. In the case of H<sub>2</sub>O, the merging procedure then also includes the adjusted UMLS values, by using the previous temporarily-merged series as a reference to adjust to.

The case of water vapor is essentially the same as for HCl, in terms of methodology and datasets used, except that one dataset, UARS MLS H<sub>2</sub>O, is added at the end, using an adjustment based on the already-adjusted HALOE series as a reference during the Oct. 1991 through May 1993 (end of UARS MLS series for H<sub>2</sub>O) time period. SAGE II H<sub>2</sub>O data were affected by a channel drift issue that led to a re-calibration of the (v6.2) dataset by comparison to averages from HALOE H<sub>2</sub>O (see *Thomason et al.*, 2004); while the impact of this issue on average SAGE II H<sub>2</sub>O values and drifts versus time may not be very large, SAGE II team members have themselves cautioned against the use of this dataset for trend studies. Moreover, the impact of volcanic aerosols (from El Chichon in 1982 and for several years after that, from Kelut in 1990, and from Mt. Pinatubo in 1991 and for 2-3 years after that) limits the amount of reliably-retrieved lower stratospheric SAGE II H<sub>2</sub>O for the earlier years and tends to accentuate variability, based on our inspection of the time series. *Thomason et al.* (2004) also refer to some issues with a dry bias in SAGE II H<sub>2</sub>O. In the end, we decided not to include the SAGE II H<sub>2</sub>O dataset into our (ev1) merged GOZCARDS results

for water vapor. The potential use of a recently reprocessed SAGE II dataset (version 7) would need to be evaluated. We note that some HALOE data in 1991-1992 were found to be anomalously low, compared to UARS MLS values and 1993 (and later) HALOE (and SAGE II) values. Screening of such low values is obtained by using a threshold based on HALOE extinction measurements for 22 hPa and higher pressures, although a few monthly values still seem somewhat anomalous in this time period, which also affects some merged values (details to be provided elsewhere).

### Note: Minor changes for HCl ESDR version ev1.01

A minor change occurred between the delivered ESDR version ev1.00 for HCl and the updated ev1.01 datasets. This has to do with the inclusion of low latitude profiles from ACE-FTS (for latitudes between 30°S and 30°N, meaning bins between 25°S and 25°N); the criterion for minimum acceptable number of values was set to 6 for generating a monthly mean for ACE-FTS data in this region for the upper stratosphere (pressures less than 10 hPa); for ev1.01, we keep this criterion, but apply it to the whole profiles, rather than just keeping the upper stratospheric portion. This change has been used for all species from ACE-FTS. The merged HCl files have therefore changed slightly in a few places/times, as a result of slightly different offsets compared to ev1.00 and slightly more data points (depending on the year), particularly in the lower stratosphere. Also, the HALOE zonal means have (recently) changed slightly for a few of the months as a result of modifications in the data screening relating to aerosol effects, as well as occasional profile "events" which have been screened out, per recommendations from HALOE team members. These profiles may contain retrieval artifacts associated with either a faulty trip-angle or constant-lockdown-angle registration (see http://haloe.gatsinc.com/user docs/index.php). These effects can bring the total number of good profiles in a monthly bin below our threshold for calculation of a GOZCARDS monthly zonal mean (from HALOE or SAGE data), namely we only use monthly means constructed from 15 profiles or more in a given latitude/pressure bin.

### Ozone

The means of deciding upon and obtaining a reference are species-dependent. For ozone data, SAGE II  $O_3$  is chosen as a robust reference (based on past studies of this high quality product); other GOZCARDS ozone datasets are generally adjusted for their offsets versus SAGE II and then averaged (where collocated points exist during an appropriate overlap time period). However, there are some subtleties in this procedure, summarized briefly here.

First, we have adjusted the UARS MLS and HALOE ozone values to the SAGE II ozone reference by using the mean (additive) offsets versus SAGE II ozone during the appropriate period of overlap, namely the 1991-1997 period appropriate for UARS MLS data records, and the 1991 to June 2000 period for HALOE (see the comments below for the 2000-2005 period). SAGE II ozone data were

converted from a density/height native retrieval grid to a mixing ratio/pressure grid, for comparison to other GOZCARDS-related datasets, for which a mixing ratio/pressure grid is a more natural choice; the latter grid is also most often used in comparisons to models. One needs temperature profiles for such a conversion, and any artifacts or anomalous variability in temperatures can therefore be transferred to the converted datasets; this was pointed out by McLinden et al. (2009) in relation to SAGE II data and the use of the NMC/NCEP temperature data in use at the time of the creation of SAGE II ozone (v6.2) data. They noted that artifacts in upper stratospheric and lower mesospheric SAGE II ozone can be introduced, especially after 2000. Moreover, significant changes in the relative fraction of sunset and sunrise occultations after mid-2000 can lead to artificial biases if one averages all the SAGE II ozone data (sunrises and sunsets), mostly again in the upper stratosphere and above, where diurnal effects become larger. We have noticed that there are indeed drifts versus HALOE ozone data in SAGE II ozone (VMR units) for this post-2000 period in the upper stratosphere above 3.2 hPa, which mainly results from anomalous NCEP temperature trends when compared to MERRA and HALOE temperature data. For the creation of a merged GOZCARDS dataset, we have, therefore, avoided the use of SAGE II data for pressures less than or equal to 3.2 hPa; instead, we use the HALOE dataset, previously adjusted to match SAGE II average values (from the 1991 to 2000 time period analysis of HALOE and SAGE II data), as a reference for this later time period. The adjustment of the Aura MLS time series vis-à-vis SAGE II is performed by using average offsets from 2004-2005 versus SAGE II ozone for pressures larger than 3.2 hPa, and versus the previously adjusted HALOE ozone dataset for smaller pressures (higher altitudes). Finally, the ACE-FTS ozone dataset is adjusted by using as an average reference the previously merged dataset from SAGE II, HALOE, and Aura MLS during the 2004-2005 overlap period used here; these results are then merged together for the final ozone dataset.

### **Notes of Caution**

There are some regions where the amount of overlap between datasets can become an issue for the proper merging of these averaged zonal means via this method. In particular, this can occur when there are also large seasonal changes, and the sampling during the overlap period is not sufficient for enough stability in the results (also, an occasional poorer quality data average could more heavily influence the end result); we noticed some significant discontinuities (offsets) between the adjusted UARS MLS and Aura MLS ozone series, notably for latitudes poleward of the 65°N or 65°S bin, in the upper stratosphere and lower mesosphere. We have omitted these regions from the final merged dataset; a later merged data version could make use of more sophisticated analyses (e.g., fits to time series) to reduce or remove such inconsistencies, and provide a somewhat more complete (global) dataset. The high latitude regions mentioned above should be treated with some caution at the stratospheric pressures (1 hPa to 215 hPa inclusive)

for which we provide merged data (and where signs of inconsistencies are less obvious by inspection).

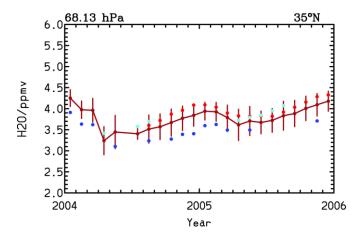
Also, for H<sub>2</sub>O, one should be cautious about some of the larger H<sub>2</sub>O mixing ratios in the upper mesosphere (typically for pressures smaller than 0.03 hPa) during the summer months in both hemispheres; these outliers (zonal mean values of about 10 ppmv or larger) are artificially high as a result of contamination of the HALOE measurements by polar mesospheric clouds (PMCs), which can affect the monthly means. These contaminated values are somewhat difficult to screen out "perfectly", but a cautionary note is in order. The same holds for the somewhat low values of lower stratospheric HALOE H<sub>2</sub>O prior to mid-1992, as mentioned above.

### **Other Species**

For somewhat simpler cases, the merging procedure consists of averaging the source datasets over the overlap time period to obtain the reference, and using the correspondingly-adjustmed series to obtain the merged series. This is true for  $N_2O$  and  $HNO_3$  for the Aura MLS and ACE-FTS common time period (Aug. 2004 onward), as well as for adjustments of HF and CH<sub>4</sub> series from HALOE and ACE-FTS during their fairly brief overlap period in 2004-2005. For other species, like ClO or  $HNO_3$ , as a large data gap exists between the UARS MLS (1991-1997) and Aura MLS (2004-current) time series, there is either no adjustment of one series versus the other, or some recommendations for adjustments will be provided at a later date, after further validation and related work.

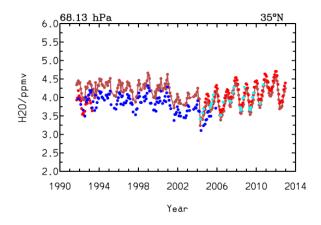
# 1.4 Sample Results

The following plots illustrate the methodology and a few sample results for several of the species intended for the first phase of deliveries for the GOZCARDS archive. The merged time series obtained for GOZCARDS attempt to be very faithful representations of the originally-produced source datasets (the properly screened zonal average series based upon the original "Level 2" set of individual profiles), meaning that no data gaps are filled (for example by fitting functions to the sparse datasets). Such fitting procedures will be up to individual users; also, model/data comparisons could be best performed by sampling the models in a way that is not continuous, but rather, follows the data record sampling in time and space.

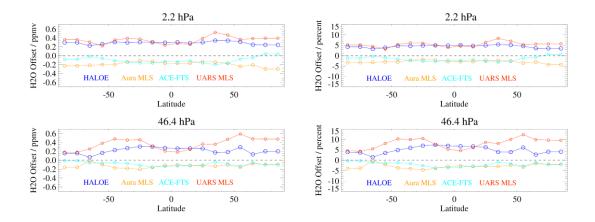


**Figure 2.** H<sub>2</sub>O monthly mean abundances versus time during the period of overlap between the satellite measurements from HALOE (blue), ACE-FTS (cyan), and Aura MLS (red) at 68 hPa for 35°N. Merged time series obtained after the merging procedure described above is given by the connected brown points.

Figure 2 shows an example of the overlap time period for H2O source datasets from HALOE, ACE-FTS, and Aura MLS, at 100 hPa in the 45°N latitude bin (covering 40°N-50°N). The resulting merged time series in this overlap period is shown (brown points). An expanded version of the (unadjusted) source datasets and the merged data record for 1991 through 2010 is shown in Figure 3, for this same latitude/pressure bin. Also, the early time period data from UARS MLS are shown; this dataset is adjusted to the original merged series for the final merged product.



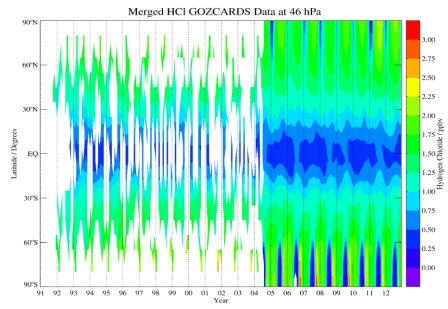
**Figure 3.** H<sub>2</sub>O monthly mean abundances from the source datasets and the resulting merged record for the same latitude/pressure bin as for Figure 2, but for the time period from 1992 through 2010. This plot also shows the UARS MLS points in 1992-1993 (red points for that time period).



**Figure 4.** Offsets applied to each of four H<sub>2</sub>O datasets (see legend in above plots) are shown versus latitude for the 2.2 hPa pressure level ((a) in ppmv and (b) in %) and for 46.4 hPa ((c) in ppmv and (d) in %). Such offsets are applied (additively, in mixing ratio units) to the original source data series to obtain adjusted series and resulting merged time series. For example, as the HALOE and UARS MLS values are drier than the mean reference, these datasets are associated with positive offsets, applied to raise their average values, whereas the opposite is true (for the cases illustrated above) for Aura MLS and ACE-FTS.

Average offsets applied to the original H<sub>2</sub>O monthy mean time series are shown in Figure 4 for two pressure levels. The sum of the offsets from HALOE, Aura MLS, and ACE-FTS equals zero, as each of these 3 series is given equal weighting in this merging procedure (during 2004-2005).

Several other examples are shown for global HCl series in the following pages. This includes a contour plot of the merged HCl field on the 46 hPa surface (Figure 5), merged and (unadjusted) source data time series for all latitudes at 46 and 1 hPa (Figures 6 and 7). Sample time series of the standard deviations for the merged monthly mean HCl record at 46 and 1 hPa are also shown in Figures 8 and 9 (derivations of these quantities will be described elsewhere). Descriptions of other quantities provided in the GOZCARDS files are summarized in section 3. These plots illustrate that different sampling and other characteristics from various instruments can lead to different views of atmospheric variability; one also needs to contend with data gaps when trying to analyze or interpret such long merged time series. Discussions of uncertainties will be provided at a later date, but the range of available zonal mean datasets can help to bound the likely ("true") absolute values. Every effort has been made to use robust and consistent datasets among the GOZCARDS ensemble considered, given the time and resources available; care has been taken not to merge datasets when significant deviations exist not just in absolute values, but also in temporal tendencies (such as trends of deseasonalized anomalies, not shown here). For example, the known issue in Aura MLS HCl for upper stratospheric trends (see Figure 7, where the red symbols do not track the expected HCl decline shown by the ACE-FTS points) implies that it would not be wise to include that dataset as part of the merged result, in order to reliably track the small decline in upper stratospheric HCl (relevant for total chlorine trends).

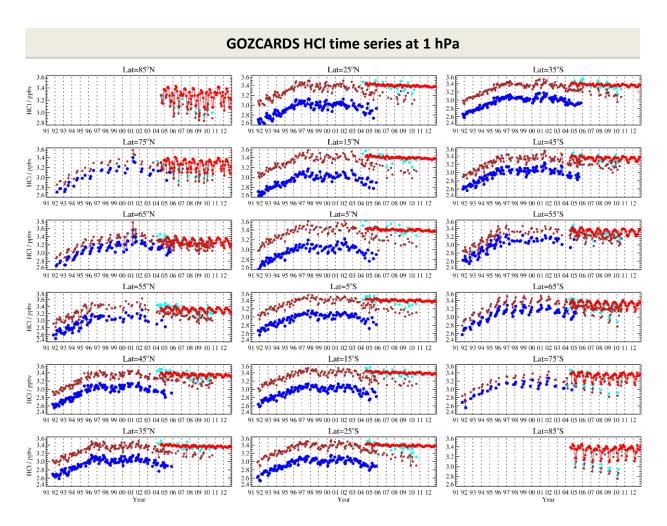


**Figure 5.** Sample GOZCARDS HCl field (ppbv) at 46 hPa (1991-2012) versus latitude. This field is obtained by combining HALOE (1991-2005), ACE-FTS (2004-2012), and Aura MLS (2004-2012) data records.

### **GOZCARDS HCl time series at 32 hPa**

### $\begin{array}{c} \textbf{HCl Data at 32 hPa} \\ \textbf{Blue= HALOE 0.82, Cyan= ACEFTS 0.83, Red= AMLS 0.81, Brown= Merged 1.01} \end{array}$ HCl/ppbv 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 Lat=75°N HCl/ppbv 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 Lat=65°N Lat=5°N Lat=55°S 0.5 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 99 00 01 02 03 04 05 06 07 08 09 10 11 12 00 01 02 03 04 05 06 07 08 09 10 11 12 Lat=55°N Lat=65°S 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 Lat=75°S Lat=45°N Lat=15°S 0.8 0.5 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 Lat=35°N Lat=25°S Lat=85°S 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12 91 92 93 94 95 96 97 98 99 00 01 02 03 04 05 06 07 08 09 10 11 12

**Figure 6.** Sample monthly mean mixing ratio (ppbv) time series from the GOZCARDS HCl data record (1991-2012) at 32 hPa. Source time series (unadjusted) are shown for HALOE (blue), ACE-FTS (cyan), and Aura MLS (red), along with the resulting merged time series (brown).



**Figure 7.** Sample monthly mean mixing ratio (ppbv) time series from the GOZCARDS HCl data record (1991-2012) at 1 hPa. Source time series (unadjusted) are shown for HALOE (blue), ACE-FTS (cyan), and Aura MLS (red), along with the resulting merged time series (brown). For pressures less than 10 hPa, only the HALOE and ACE-FTS HCl fields are used, although the average offsets and adjustments for HALOE and ACE-FTS time series were also derived using Aura MLS for this upper stratospheric region. This is because HCl trends from Aura MLS in the upper stratosphere are not reliably captured (as the Aura MLS HCl decrease in this region is too slow); the primary HCl band from Aura MLS has not been used continuously after April 2006, as a result of hardware degradation for this band.

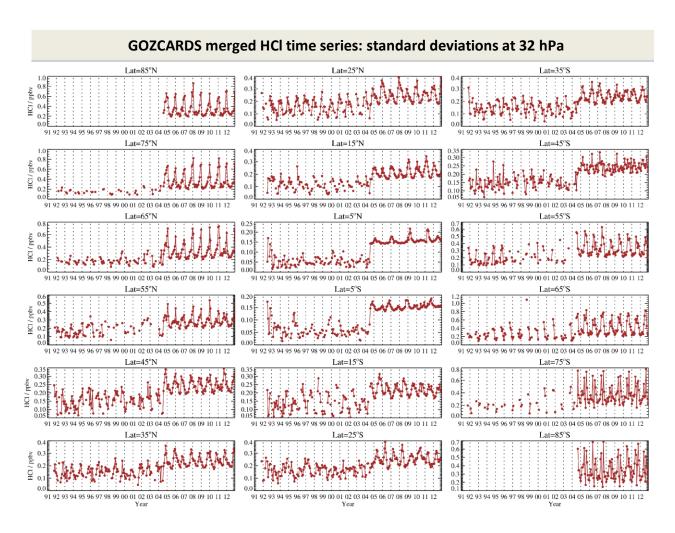


Figure 8. Sample standard deviations (ppbv) from the GOZCARDS merged HCl data record at 32 hPa.

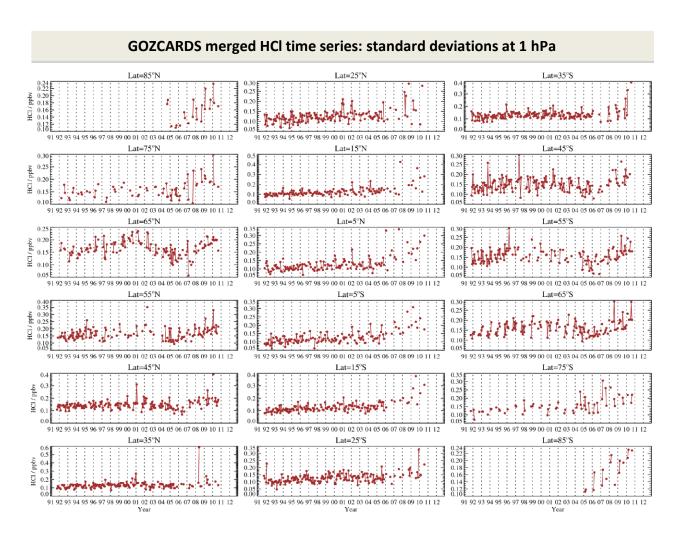
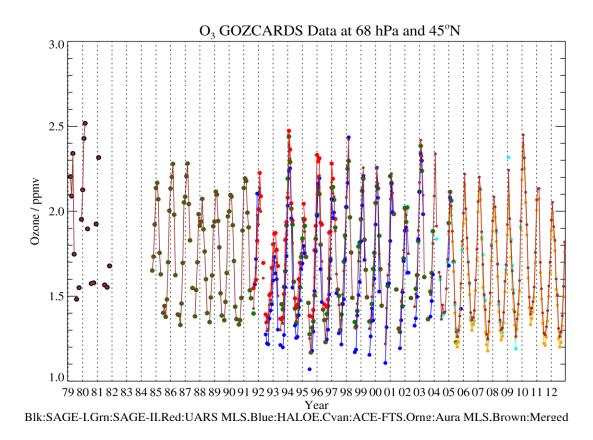
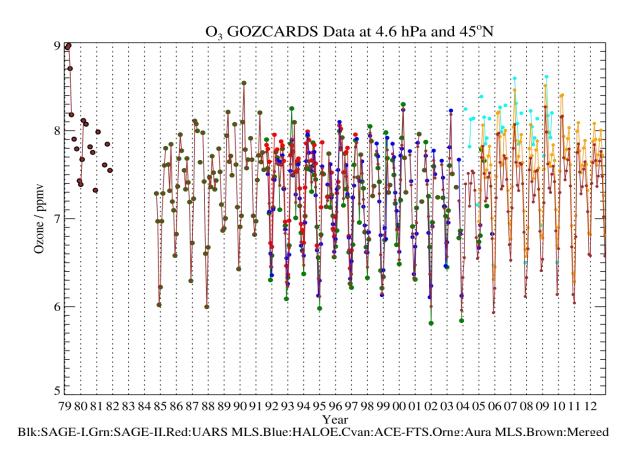


Figure 9. Sample standard deviations (ppbv) from the GOZCARDS merged HCl data record at 1 hPa.

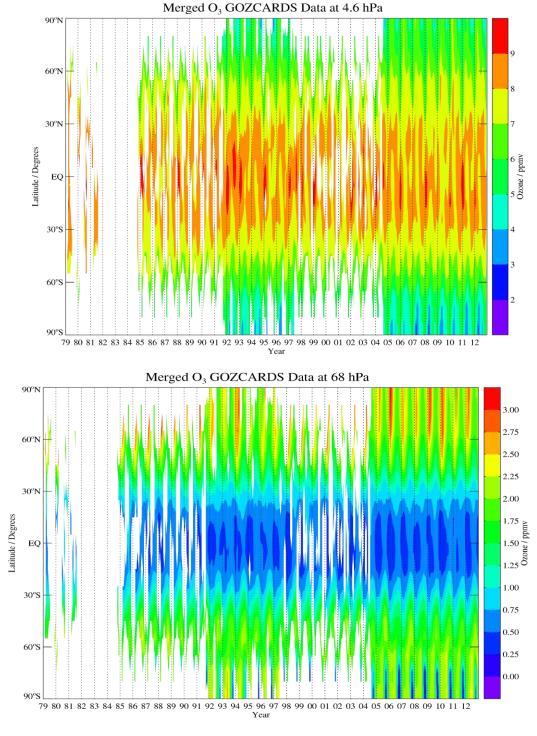
The following two plots show sample time series for the GOZCARDS ozone record at 40°N-50°N (Figure 10 for the lower stratosphere and Figure 11 for the upper stratosphere), with all source datasets and merged datasets. Validation of this sort of dataset includes internal validation (as the merged time series generally track the source datasets quite faithfully, except for some offsets), and we have also performed comparisons to other long-term datasets (to be discussed elsewhere), with overall good results; this also holds for water vapor datasets. Figure 12 shows sample contour plots of the merged ozone field (latitude/time views for specific pressure levels).



**Figure 10.** Sample GOZCARDS ozone time series from 1979 through 2012 at 68 hPa and 45°N. SAGE-I (source) data are shown in black (under the merged brown values), and SAGE-II, HALOE, UARS MLS, ACE-FTS, and Aura MLS source data points are shown in green, blue, red, cyan, and orange, respectively. The merged (brown) dataset is a subset of the GOZCARDS ozone profile ESDR.

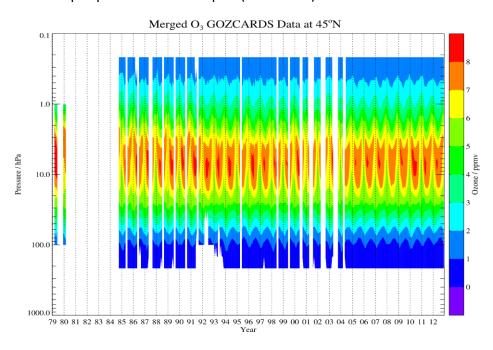


**Figure 11.** Sample GOZCARDS ozone time series (source data and merged data) from 1979 through 2012 at 4.6 hPa and 45°N; the various datasets are identified by color, as described in the previous Figure.

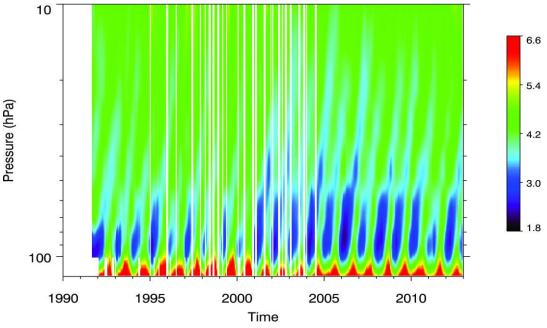


**Figure 12.** Sample GOZCARDS merged ozone fields (ppmv) at 4.6 hPa (top panel) and 68 hPa (bottom panel) as a function of latitude and time, from 1979 through 2012.

Figure 13 displays a sample contour plot (pressure/time view) for the merged ozone field at 40°N-50°N, and Figure 14 shows a similar view, but for the "tape recorder" features of the merged water vapor product in the tropics (20°S-20°N).



**Figure 13**. Sample contour plot for the GOZCARDS merged ozone field (ppmv) from the 45°N latitude bin (40°N-50°N average) as a function of pressure and time (1979-2012).



**Figure 14**. GOZCARDS merged water vapor "tape recorder" contour plot; average H₂O mixing ratio (ppmv) for 20°S-20°N from Oct. 1991 through 2012.

Figure 15 shows the GOZCARDS N<sub>2</sub>O field at two pressure levels for 2004-2012, using a merged product from Aura MLS and ACE-FTS data (starting in August 2004 and ending in Dec. 2012).

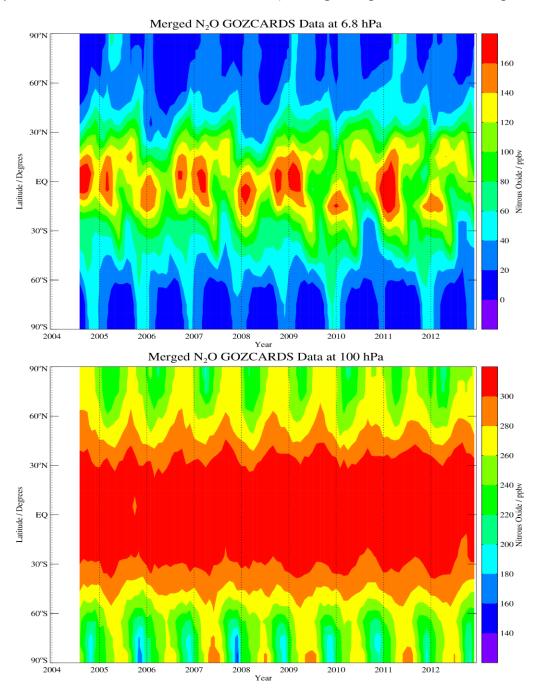
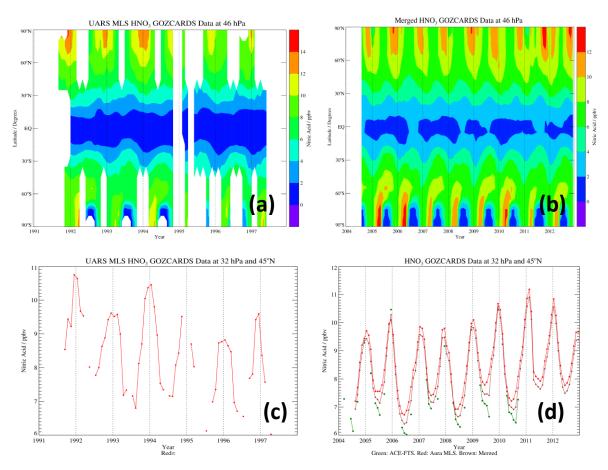


Figure 15. Sample GOZCARDS merged  $N_2O$  fields (ppbv) at 6.8 hPa (top panel) and 100 hPa (bottom panel) as a function of latitude and time, from Aug. 2004 through 2012. This dataset includes Aura MLS and ACE-FTS  $N_2O$  data.

Figure 16 (top two panels) shows the GOZCARDS HNO<sub>3</sub> field at 46 hPa from the UARS time period (1991-1997) and the separate 2004-2012 period, for which a merged product was produced (as for N<sub>2</sub>O above) using Aura MLS and ACE-FTS data; also shown (bottom two panels) are time series for 45N and 32 hPa from both these periods (the bottom right panel includes the source and merged series). Adjustments are in order in terms of the HNO<sub>3</sub> cross-calibration for these two separate time periods. We have investigated this to some extent and believe that small adjustments to the UARS MLS HNO<sub>3</sub> field are a likely outcome, based on a consideration of ground-based (FTIR) column HNO<sub>3</sub> data covering the full time period (and the fact that Aura MLS and ACE-FTS HNO<sub>3</sub> data tend to match ground-based and other correlative data quite well); obtaining an optimum global set of (fairly small) adjustments for the UARS MLS HNO<sub>3</sub> field requires more work and will be limited by the number of sites/locations with such ground-based data, as well as the different vertical resolutions of these datasets. More ongoing collaborative work regarding such analyses is needed.



**Figure 16.** Sample time series for GOZCARDS records of stratospheric HNO<sub>3</sub> (ppbv). (a) Contour plot (latitude/time) at 46 hPa from UARS MLS HNO<sub>3</sub> data records for 1991-1997 (b) Contour plot (latitude/time) at 46 hPa from merged Aura MLS and ACE-FTS HNO<sub>3</sub> data for 2004-2012 (c) Time series from UARS MLS HNO<sub>3</sub> data at 45°N and 32 hPa for 1991-1997 (d) Time series from merged Aura MLS and ACE-FTS HNO<sub>3</sub> data at 45°N and 32 hPa for 2004-2012.

### 1.5 Data Disclaimer

One should note that the merged time series obtained for GOZCARDS are intended to be quite faithful representations of the originally-produced source datasets (the properly screened zonal average series based upon the original "Level 2" set of individual profiles), meaning that no data gaps are filled, for example by fitting functions to the sparse datasets. Such fitting procedures will be up to individual users; also, model/data comparisons could be best performed by sampling the models in a way that is not continuous, but rather, follows the data record sampling in time and space.

# 2. Data Organization

The data records consist of zonal means for one year's worth of data. These files contain all data available to GOZCARDS for the given year.

# 2.1 File Naming Convention

The GOZCARDS data product files are named according to the following convention:

GOZ-<data\_type>-<type\_code >\_<product >\_<esdr\_version>\_<year>.nc4

### where:

- Data\_type = The type of data being presented. There are two types: "Source" for source data values and "Merged" for the merged data values.
- Type\_code = The processing options, a 3 letter code where each letter stands for an option in the GOZCARDS data reporting.
  - o Character 1: Time granularity. Values are "M" for monthly, and "D" for daily.
  - Character 2: Latitude coordinate. Values are "L" for geodetic latitude, "E" for equivalent latitude.
  - Character 3: Vertical coordinate. Values are "P" for pressure and "T" for potential temperature (theta).
- Product = The data product i.e. "HCl", "O3", etc...
- ESDR Version = The version of the processed GOZCARDS ESDR in the format evX-XX.
- Year = The 4 digit year of the data.

### Filename example:

GOZ-Source-MLP\_HCl\_ev1-00\_2010.nc4

(for the first likely data version number, which would be referred to as ev1.00, or ev1 for short).

## 2.2 File Format and Structure

GOZCARDS data files are written in NetCDF4 (<a href="http://www.unidata.ucar.edu/software/netcdf/">http://www.unidata.ucar.edu/software/netcdf/</a>). These files house all of the science data fields described in the rest of this section. Within each file there is also a set of global attributes that define the metadata for that data product. Section 3.0 of this document describes the dimensions, global attributes, and data fields in detail.

# 2.3 Key Science Data Fields

The GOZCARDS science data are organized by chemical species or temperature into two main product types:

- **Source products**, which contain zonal means and related information, calculated from original ('Level 2' type) satellite instruments and products.
- **Merged products**, which contain zonal means and related information, calculated as a result of a merging process that ties together the source datasets, after bias removal and averaging.

The key data fields are organized according to product, with various groupings within the files; in particular, each instrument's dataset for a given product is grouped by instrument in each source file for that product. The names below identify the key science data fields. Note that a merged product (or product plan) does not always exist; in particular, there is no merged product planned for CIO (or CIOx), as there is a large data gap between two different instruments' time series, and no recommended/planned adjustments to the zonal mean source datasets. Also, the MERRA-based zonal mean temperature GOZCARDS product is provided/planned as a source dataset, with no corresponding merged dataset.

### **Product Short Name Convention**

The list of short names that apply to each product's file set is as described below. A sample name for the data files making up the MEaSURES GOZCARDS ESDR is GOZSmlpHCl.

The character index meaning is as follows:

```
1-3 = Goz (short for NASA MEaSUREs project name = GOZCARDS)
```

4 = S or M for Source or Merged product/file

5 = m or d for time axis (m = monthly, or d = daily)

6 = I (for x-axis = latitude)

7 = p (for y-axis = pressure)

8-\* = Product Name (e.g., HCl)

**Table 2.1.** GOZCARDS Monthly Source Data Products. Products shown in blue have been made publicly available.

Short Name	Long Name
GozSmlpHCl	GOZCARDS Source Data for Hydrogen Chloride Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpH2O	GOZCARDS Source Data for Water Vapor Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpO3	GOZCARDS Source Data for Ozone Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpClO	GOZCARDS Source Data for Chlorine Monoxide Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpHNO3	GOZCARDS Source Data for Nitric Acid Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpHF	GOZCARDS Source Data for Hydrogen Fluoride Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpN2O	GOZCARDS Source Data for Nitrous Oxide Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpCH4	GOZCARDS Source Data for Methane Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpClOx	GOZCARDS Source Data for Chlorine Oxide Radicals Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpNO2	GOZCARDS Source Data for Nitrogen Dioxide Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpNO	GOZCARDS Source Data for Nitric Oxide Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpNOx	GOZCARDS Source Data for Nitrogen Oxide Radicals Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid
GozSmlpT	GOZCARDS Source Data for Temperature Monthly Zonal Averages on a Geodetic Latitude and Pressure Grid

**Table 2.2.** GOZCARDS Monthly Merged Data Products. Products shown in blue have been made publicly available.

Short Name	Long Name		
GozMmlpHCl	GOZCARDS Merged Data for Hydrogen Chloride Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		
GozMmlpH2O	GOZCARDS Merged Data for Water Vapor Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		
GozMmlpO3	GOZCARDS Merged Data for Ozone Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		
GozMmlpHNO3	GOZCARDS Merged Data for Nitric Acid Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		
GozMmlpHF	GOZCARDS Merged Data for Hydrogen Fluoride Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		
GozMmlpN2O	GOZCARDS Merged Data for Nitrous Oxide Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		
GozMmlpCH4	GOZCARDS Merged Data for Methane Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		
GozMmlpNO2	GOZCARDS Merged Data for Nitrogen Dioxide Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		
GozMmlpNO	GOZCARDS Merged Data for Nitric Oxide Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		
GozMmlpNOx	GOZCARDS Merged Data for Nitrogen Oxide Radicals Monthly Zonal Averages on a		
	Geodetic Latitude and Pressure Grid		

**Table 2.3.** GOZCARDS Daily Source Data Products.

Short Name	Long Name
GozSdlpHCl	GOZCARDS Source Data for Hydrogen Chloride Daily Zonal Averages on a
-	Geodetic Latitude and Pressure Grid
GozSdlpH2O	GOZCARDS Source Data for Water Vapor Daily Zonal Averages on a
	Geodetic Latitude and Pressure Grid
GozSdlpO3	GOZCARDS Source Data for Ozone Daily Zonal Averages on a
	Geodetic Latitude and Pressure Grid
GozSdlpHNO3	GOZCARDS Source Data for Nitric Acid Daily Zonal Averages on a
	Geodetic Latitude and Pressure Grid
GozSdlpN2O	GOZCARDS Source Data for Nitrous Oxide Daily Zonal Averages on a
	Geodetic Latitude and Pressure Grid
GozSdlpClO	GOZCARDS Source Data for Chlorine Daily Monthly Zonal Averages on a
	Geodetic Latitude and Pressure Grid
GozSdlpClOx	GOZCARDS Source Data for Chlorine Oxide Radicals Daily Monthly Zonal Averages on
	a Geodetic Latitude and Pressure Grid
GozSdlpT	GOZCARDS Source Data for Temperature Daily Zonal Averages on a
	Geodetic Latitude and Pressure Grid

Table 2.3 above lists the daily products (in yearly files) that are expected from the MLS suite of measurements, mostly from the Aura MLS continuous dataset (from August 2004 onward). There is no merging process involved in this set of products, although one could apply the offsets from the monthly file offset values to the daily MLS products if this is judged to be desirable for a particular application. For some applications, MLS daily zonal averages on a vertical and latitude grid equal to (or closer to) the original MLS retrieval grid may be (viewed as) more useful. The MLS team should be contacted separately by individuals interested in such special products.

## 3. Data Contents

## 3.1 Group information

GOZCARDS files contain source data or merged data (for Source and Merged files respectively) stored as NetCDF4 groups. The available groups (instruments) for each source dataset can be

determined by looking at Table 1. Only active data sources will be included for a given year. Merged data records will typically only have one group.

### 3.2 Global Attributes

In addition to the data values, a full suite of metadata/attributes is supplied with each dataset. Some metadata are required by standard conventions, some are there to meet data provenance requirements, and others are provided as a convenience to users of the GOZCARDS products.

**Table 3.1.** Global attributes in a GOZCARDS data granule.

Name	Type	Description
Conventions	String	The CF conventions used in the file.
GranuleID	String	The name of the file/granule
ProductionDateTime	String	When the data file was produced
identifier_product_doi	String	The Digital Object Identifier or DOI (e.g. 10.5067/MEASURES/GOZCARDS/DATAxyzw)
identifier_product_doi_authority	String	The authority responsible for the DOI ( <a href="http://dx.doi.org">http://dx.doi.org</a> )
Format	String	The format of the file
SizeBytesDataGranule	String	The size of the file when first written
RangeBeginningDate	String	The first possible date of data used
RangeBeginningTime	String	The first possible time of the first date used
RangeEndingDate	String	The last possible date of data used.
RangeEndingTime	String	The last possible time of the last date used.
ContactPersonName	String	Name of responsible person(s)
ContactPersonRole	String	The contact person's role in this MEaSUREs project.
ContactPersonEmail	String	The contact person's email address.
ContactPersonAddress	String	The contact person's physical address
RelatedURL	String	Website containing further information on the project.
ObservationArea	String	The viewing area i.e. Global

ProcessingDate	String	The date the data was produced
ProcessingCenter	String	Where the data was produced
InputOriginalFile	String	The name(s) of the original data files used or equivalent.
ProductGenerationAlgorithm	String	Reference to where algorithms can be found
ProductGenerationAlgorithmVersion	String	The version of the algorithm
ProductReference	String	Reference to where the product notes can be found
SouthBoundingCoordinate	Float	Southernmost Latitude (-90 degrees)
NorthBoundingCoordinate	Float	Northernmost Latitude (90 degrees)
LatitudeResolution	Float	The resolution of the bins
EastBoundingCoordinate	Float	East Bounding Coordinate (180 degrees)
WestBoundingCoordinate	Float	West Bounding Coordinate (180 degrees)
LongitudeResolution	Float	The resolution (zonal mean=360 degrees)
ShortName	String	The short name of the product
LongName	String	The long name of the product
DataProduct	String	The data product
LatitudeType	String	The type of latitude coordinate (geodetic, equivalent)
LevelType	String	The type of vertical coordinate (pressure, potential temperature)
TimeResolution	String	The resolution of the data (monthly, daily)
History	String	An audit trail of changes to this dataset.

# 3.3 Group Attributes

A secondary class of metadata in a GOZCARDS file resides in each group. This metadata describes the individual dataset defined in the file. This includes data source and version information.

**Table 3.2.** Attributes in a GOZCARDS group.

Name	Type	Description
OriginalFileVersion	String	The version of the original data. For groups of a source dataset, this = data versions, and in a merged file group, this = GOZCARDS Earth Science Data Record version.
OriginalFileProcessingCenter	String	Where the data used was processed
DataQuality	String	Statement on what data screening is being used.
DataSource	String	The original data source (instrument/model for source files, a list of instrument and versions for merged files)
DataSubset	String	Any subset of the original data (e.g., daytime data).

## 3.4 Dimensions

There are two different GOZCARDS data group structures, one for the source files and one for the merged files. Variables are organized into group structures by instrument/source, (e.g. SAGE2, HALOE, AMLS, MERRA, etc...). Variables have the same names within groups or across products. Each variable also contains a set of attributes.

Table 3.3. Dimensions associated with the GOZCARDS dataset.

Name	Description
lat	The number of latitude bins in the dataset.
lev	The number of vertical levels in the dataset.
time	The number of time periods in the dataset
day_in_month	The maximum number of days in a month.
	(Monthly instrument source files only)
data_source	The number of data sources used (Merged files only)
overlap	The number of overlap periods used (Merged files only)
max_string_length	The length of strings (Merged files only)

## 3.5 Variables

There are two different GOZCARDS data group structures, one for the source files and one for the merged files. Variables are organized into group structures by instrument/source, (e.g. SAGE2, HALOE, AMLS, MERRA, etc...). Variables have the same names within groups or across products. Each variable also contains a set of attributes.

#### 3.5.1 Source Product Variables

**Table 3.4.** Variables in merged GOZCARDS data records.

Name	Data Type (Dimensions)	Description
lat	Float(lat)	The center latitude for each bin in degrees.
lev	Float(lev)	The vertical level of the data.
time	Int(time)	The day number with respect to the reference; for monthly files, the 15 <sup>th</sup> day of the month. The reference day number is Jan. 1, 1950.
day_in_month	Int(day_in_month)	The day of the month.
average	Float(time, lat, lev)	The average value of data in each bin.
nvalues	Int(time, lat, lev)	The number of data values in each bin.
std_dev	Float(time, lat, lev)	The standard deviation of data values in each bin.
std_error	Float(time, lat, lev)	The standard error of data values in each bin.
rms_uncertainty	Float(time, lat, lev)	The RMS uncertainty of data values in each bin.
minimum	Float(time, lat, lev)	The minimum data value in each bin.
maximum	Float(time, lat, lev)	The maximum data value in each bin.
lat_avg	Float(time, lat, lev)	The average latitude of data values in each bin.
lat_min	Float(time, lat, lev)	The minimum latitude of data values in each bin.
lat_max	Float(time, lat, lev)	The maximum latitude of data values in each bin.
lst_avg	Float(time, lat)	The average local solar time of data values in each bin (height-independent).
lst_min	Float(time, lat)	The minimum local solar time of data values in each bin.

lst_max	Float(time, lat)	The maximum local solar time of data values in each bin.
sza_avg	Float(time, lat)	The average solar zenith angle of data values in each bin.
sza_min	Float(time, lat)	The minimum solar zenith angle of data values in each bin.
sza_max	Float(time, lat)	The maximum solar zenith angle of data values in each bin.
days_used	Byte(time, lev, lat, day_in_month) for monthly files. Byte(time, lev, lat) for daily files.	A bitmask indicating the days when data is used in each bin.  1 = data is used  0 = no data is used

## 3.5.2 Merged Product Variables

**Table 3.5.** Variables in merged GOZCARDS data records.

Name	Data Type (Dimensions)	Description
lat	Float(lat)	The center latitude for each bin in degrees.
lev	Float(lev)	The vertical level of the data.
time	Int(time)	The day number with respect to the reference; for monthly files, the 15 <sup>th</sup> day of the month. The reference day number is Jan. 1, 1950.
data_source	Int(data_source)	Index of data sources (e.g., 1, 2,)
overlap	Int(overlap)	Index of overlap period(s) (e.g., 1, 2,)
data_source_name	Char(data_source, max_string_length)	The string representation of each source dataset used in the merge; e.g., 'HALOE v19'.
overlap_start_date	Int(overlap)	The starting date of each overlap period (same units as 'time').
overlap_end_date	Int(overlap)	The ending date of each overlap period (same units as 'time').
overlap_used_source	Byte(overlap, data_source)	A bitmask indicating if a given data source is used in each overlap period: 0 = not used or no adjustment, 1 = used, 2 = previously adjusted source dataset is used again (in another period, to merge another dataset).
overlap_source_total	Int(overlap, data_source, lev, lat)	The total number of (time series) values from each data source used in each overlap period in each bin.
Average	Float(time, lat, lev)	The merged value of data.
nvalues	Int(data_source, time, lat, lev)	The number of useful data values found in each bin for each source dataset used in the merge.
std_dev	Float(time, lat, lev)	The standard deviation of the merged data ("average").
std_error	Float(time, lat, lev)	The standard error of the merged data ("average").
minimum	Float(time, lat, lev)	The minimum (zonal mean) data value from all source datasets in each bin.
maximum	Float(time, lat, lev)	The maximum (zonal mean) data value from all source

		datasets in each bin.
offset	Float(data_source, lat, lev)	The additive (average) offset applied to each source dataset (series) to obtain the merged value in each bin.
offset_std_error	Float(data_source, lat, lev)	The standard error of the (average) offset values above.

## 3.5.3 Variable Attributes

**Table 3.6.** Variable attributes for all GOZCARDS data fields.

Name	Data Type	Description
_FillValue	Float	Value used to identify missing (or bad) data. Set to -999.0.
long_name	String	Ad hoc description of the variable.
description	String	The description of the variable.
units	String	The units of the variable.

# 4. Options for Reading the Data

There are many tools and visualization packages (free and commercial) for viewing and dumping the contents of netCDF4 files. Libraries are available in several programming languages for writing software to read netCDF4 files. A few simple to use command-line and visualization tools, as well as programming languages for reading the GOZCARDS data files are listed in the sections below. For a comprehensive list of netCDF tools and software, please see

http://www.unitdata.ucar.edu/software/netcdf/.

### 4.1 Command Line Utilities

#### 4.1.1 ncdump (free)

The ncdump tool, developed by Unidata, will print the contents of a netCDF or compatible file to standard out as CDL text (ASCII) format. The tool may also be used as a simple browser, to display the dimension names and lengths; variable names, types, and shapes; attribute names and values; and optionally, the values of data for all variables or selected variables. The ncdump tool is included with the netCDF library.

http://www.unidata.ucar.edu/downloads/netcdf/

### 4.1.2 h5dump (free)

Since netCDF4 is built on HDF5, the h5dump tool, developed by the HDFGroup, can also be used to examine the contents of netCDF4 files and dump their contents, in human readable form, to an ASCII file, or alternatively to an XML file or binary output. It can display the contents of the entire HDF5 file or selected objects, which can be groups, datasets, a subset of a dataset, links, attributes, or datatypes. The h5dump tool is included as part of the HDF5 library, or separately as a stand-alone binary tool at:

http://www.hdfgroup.org/HDF5/release/obtain5.html

### 4.2 Visualization Tools

## 4.2.1 Panoply (free)

Panoply, developed at the Goddard Institute for Space Studies (GISS), is a cross-platform application which plots geo-gridded arrays from netCDF, HDF and GRIB dataset required. The tool allows one to slice and plot latitude-longitude, latitude-vertical, longitude-vertical, or time-

latitude arrays from larger multidimensional variables, combine two arrays in one plot by differencing, summing or averaging, and change map projections. One may also access files remotely into the Panoply application.

http://www.giss.nasa.gov/tools/panoply/

#### 4.2.2 HDFView (free)

HDFView, developed by the HDFGroup, is a Java-based graphic utility designed for viewing and editing the contents of HDF4 and HDF5 files. It allows users to browse through any HDF file, starting with a tree view of all top-level objects in an HDF file's hierarchy. HDFView allows a user to descend through the hierarchy and navigate among the file's data objects. Editing features allow a user to create, delete, and modify the value of HDF objects and attributes. For more info see:

http://www.hdfgroup.org/hdf-java-html/hdfview/

## 4.3 Programming Languages

Advanced users may wish to write their own software to read netCDF4 data files. The following is a list of available netCDF4 programming languages:

#### Free:

C/C++ (http://www.unidata.ucar.edu/software/netcdf/)

Fortran (<a href="http://www.unidata.ucar.edu/software/netcdf/">http://www.unidata.ucar.edu/software/netcdf/</a>)

Java (http://www.unidata.ucar.edu/software/netcdf/software.html#Java%20interface)

Python (http://www.unidata.ucar.edu/software/netcdf/software.html#Python)

Perl (http://www.unidata.ucar.edu/software/netcdf/software.html#Perl)

#### Commercial:

IDL (<a href="http://www.unidata.ucar.edu/software/netcdf/software.html#IDL">http://www.unidata.ucar.edu/software/netcdf/software.html#IDL</a>)

Matlab (<a href="http://www.unidata.ucar.edu/software/netcdf/software.html#MATLAB">http://www.unidata.ucar.edu/software/netcdf/software.html#MATLAB</a>)

## 5. Data Services

### 5.1 Mirador

The GES DISC provides basic temporal and advanced (event) searches through its Mirador search and download engine:

#### http://mirador.gsfc.nasa.gov/

Mirador offers various download options that suit users with different preferences and different levels of technical skills. Users can start from a point where they don't know anything about these particular data, its location, size, format, etc., and quickly find what they need by just providing relevant keywords, such as a data product (e.g. "GozMmlpHCl"), or a parameter such as "ozone".

#### 5.2 OPeNDAP

The Open Source Project for a Network Data Access Protocol (OPeNDAP) provides remote access to individual variables within datasets in a form usable by many OPeNDAP enabled tools, such as Panoply, IDL, Matlab, GrADS, IDV, McIDAS-V, and Ferret. Data may be subsetted dimensionally and downloaded in an ASCII, netCDF3 or binary (DAP) format. The GES DISC offers the SBUV MZM data products through OPeNDAP.

http://measures.gsfc.nasa.gov/opendap/GOZCARDS/

### 5.3 Reverb

Reverb is the next generation metadata and service discovery tool for NASA's Earth science data including EOSDIS datasets and granules. Through the Reverb web interface users can enter keyword, spatial and temporal information to search the Earth Observing System (EOS) Clearinghouse (ECHO) system, a spatial and temporal metadata registry and data broker. Data orders submitted through Reverb will be transmitted to the corresponding data center for processing.

http://reverb.echo.nasa.gov/

## 6. More Information

## 6.1 Web Resources

For other related trace gas data, please search NASA's Global Change Master Directory at <a href="http://gcmd.nasa.gov">http://gcmd.nasa.gov</a>.

## 6.2 Points of Contact

#### **GES DISC Help Desk**

URL: http://disc.gsfc.nasa.gov/

E-mail: gsfc-help-disc@lists.nasa.gov

Phone: 301-614-5224

Fax: 301-614-5228

Address: Goddard Earth Sciences Data and Information Services Center

Attn: Help Desk Code 610.2

NASA Goddard Space Flight Center

Greenbelt, MD 20771, USA

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#### **GOZCARDS** team participants

The GOZCARDS project work has primarily involved the following institutions and individuals Jet Propulsion Laboratory: Lucien Froidevaux, Ryan Fuller, Michael Schwartz, Michelle Santee, Nathaniel Livesey

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Georgia Institute of Technology: Ray Wang, Derek Cunnold

University of Maryland, College Park: Ross Salawitch, Timothy Canty

Old Dominion University: Peter Bernath

University of Toronto (Toronto, Canada): Kaley Walker

Istituto Nazionale di Geofisica e Vulcanologia (Rome, Italy): Irene Fiorucci, Giovanni Muscari

University of Edinburgh (Edinburgh, Scotland): Hugh Pumphrey

The use of MERRA data from GMAO is also acknowledged.

#### **GOZCARDS** website (at JPL)

There is also a website at the Jet Propulsion Laboratory for this MEaSUREs GOZCARDS project.

Please see <a href="http://gozcards.jpl.nasa.gov">http://gozcards.jpl.nasa.gov</a>.

The plan is for this site to provide links for the GOZCARDS data access, GOZCARDS data updates and some plot samples and user support (depending on available resources), along with pointers to future GOZCARDS data updates and GOZCARDS-related publications.

## 6.3 GOZCARDS Data Usage / Acknowledgements

The GOZCARDS datasets have been produced with care, but refinements or changes are to be expected (e.g., using a new instrument data versions, or for other types of improvements or corrections). The GOZCARDS team appreciates community involvement and feedback in this regard. Feel free to contact the GOZCARDS PI (see above) for data-related questions or discussions.

If you intend to use the dataset as part of a manuscript or planned publication, please include at least an acknowledgment to the GOZCARDS team or, for more specifics regarding co-authorship, please contact the GOZCARDS PI.

DOI reference: The GOZCARDS data record will have a DOI identifier associated with each data product (see the product name list in Table 2.1). This dataset can/should also be referenced by using the relevant DOI value from the global attribute for DOI (see Table 3.1).

# 7. Acknowledgements

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